FILE 'HOME' ENTERED AT 06:58:50 ON 16 NOV 2006

```
=> file .nash
=> s (bruton## tyrosine kinase or ATK or BPK or emk) and crystal? and x-ray
L1            0 FILE MEDLINE
L2            6 FILE CAPLUS
L3            4 FILE SCISEARCH
L4            0 FILE LIFESCI
L5            0 FILE BIOSIS
L6            5 FILE EMBASE

TOTAL FOR ALL FILES
L7           15 (BRUTON## TYROSINE KINASE OR ATK OR BPK OR EMK) AND CRYSTAL?
                AND X-RAY

=> dup rem l7
PROCESSING COMPLETED FOR L7
L8           13 DUP REM L7 (2 DUPLICATES REMOVED)

=> d ibib abs 1-13
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L8 ANSWER 1 OF 13 EMBASE COPYRIGHT (c) 2006 Elsevier B.V. All rights reserved on STN

ACCESSION NUMBER: 2005353681 EMBASE Full-text
TITLE: Global rigid body modeling of macromolecular complexes against small-angle scattering data.
AUTHOR: Petoukhov M.V.; Svergun D.I.
CORPORATE SOURCE: D.I. Svergun, European Molecular Biology Laboratory, Hamburg, Germany. svergun@embl-hamburg.de
SOURCE: Biophysical Journal, (2005) Vol. 89, No. 2, pp. 1237-1250.
Refs: 62
ISSN: 0006-3495 CODEN: BIOJAU
COUNTRY: United States
DOCUMENT TYPE: Journal; Article
FILE SEGMENT: 004 Microbiology
027 Biophysics, Bioengineering and Medical Instrumentation
LANGUAGE: English
SUMMARY LANGUAGE: English
ENTRY DATE: Entered STN: 9 Sep 2005
Last Updated on STN: 9 Sep 2005

AB New methods to automatically build models of macromolecular complexes from high-resolution structures or homology models of their subunits or domains against x-ray or neutron small-angle scattering data are presented. Depending on the complexity of the object, different approaches are employed for the global search of the optimum configuration of subunits fitting the experimental data. An exhaustive grid search is used for hetero- and homodimeric particles and for symmetric oligomers formed by identical subunits. For the assemblies or multidomain proteins containing more then one subunit/domain per asymmetric unit, heuristic algorithms based on simulated annealing are used. Fast computational algorithms based on spherical harmonics representation of scattering amplitudes are employed. The methods allow one to construct interconnected models without steric clashes, to account for the particle symmetry and to incorporate information from other methods, on distances between specific residues or nucleotides. For multidomain proteins, addition of missing linkers between the domains is possible. Simultaneous fitting of multiple scattering patterns from subcomplexes or deletion mutants is incorporated. The efficiency of the methods is illustrated by their application to complexes of different types in several simulated and practical examples. Limitations and possible ambiguity of rigid body modeling are discussed and simplified docking criteria are provided to rank multiple models. The methods described are implemented in publicly available computer programs running on major hardware platforms. .COPYRGT. 2005 by the Biophysical Society.

L8 ANSWER 2 OF 13 EMBASE COPYRIGHT (c) 2006 Elsevier B.V. All rights reserved on STN

ACCESSION NUMBER: 2005166146 EMBASE Full-text
TITLE: Hit to lead success stories - IBC Conference. Effective chemistry strategies for reducing attrition rates and speeding lead compounds into the pipeline: 31 January - 1 Frebruary 2005, San Diego, CA, USA.
AUTHOR: Nestler H.P.
CORPORATE SOURCE: H.P. Nestler, Aventis Pharmaceuticals Germany, Industrial Park Hoechst, Building G 879, D-65926 Frankfurt am Main,

Frankfurt, Germany. peter.nestler@sanofi-aventis.com
SOURCE: IDrugs, (2005) Vol. 8, No. 3, pp. 206-208. .
ISSN: 1369-7056 CODEN: IDRUFN
COUNTRY: United Kingdom
DOCUMENT TYPE: Journal; Conference Article
FILE SEGMENT: 017 Public Health, Social Medicine and Epidemiology
029 Clinical Biochemistry
030 Pharmacology
037 Drug Literature Index
LANGUAGE: English
SUMMARY LANGUAGE: English
ENTRY DATE: Entered STN: 28 Apr 2005
Last Updated on STN: 28 Apr 2005

AB The conference highlighted and elaborated on the current challenges in lead discovery, stimulating lively discussions on concepts that are likely to have an impact on drug discovery approaches. It will be interesting to observe how the field develops over the next five years. The results presented at the meeting were encouraging for a brighter 'productivity forecast' and an increased drug development success rate. .COPYRGT. The Thomson Corporation.

L8 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 2005:314583 CAPLUS Full-text
DOCUMENT NUMBER: 143:37483
TITLE: Oxidative condensation reactions of (diethylenetriamine)cobalt(III) complexes with substituted bis(pyridin-2-yl)methane ligands
AUTHOR(S): Zhou, Xiangting; Hockless, David C. R.; Willis, Anthony C.; Jackson, W. Gregory
CORPORATE SOURCE: School of Physical, Environmental, Mathematical and Physical Sciences, Chemistry, University College, The University of New South Wales, Australian Defence Force Academy, Canberra, ACT 2600, Australia
SOURCE: Journal of Molecular Structure (2005), 740(1-3), 91-100
CODEN: JMOSB4; ISSN: 0022-2860
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:37483

AB The synthesis and characterization of Co(III) complexes derived from a condensation reaction with a central or terminal N of a dien ligand and the α-C of a range of substituted bis(pyridin-2-yl)methane ligands are described. Aerial oxidation of bis(pyridin-2-yl)methane (bpm) with Co(II)/dien or direct reaction with Co(dien)Cl3 provided in low yield a single C-N condensation product [Co(dienbpm)Cl]ZnCl4 (1) (at the primary terminal NH2) after the pyridyl -CH2- is formally oxidized to -CH+-. The Me substituted ligand bpe {1,1-bis(pyridin-2-yl)ethane} behaves likewise, except both terminal (prim) and central (sec) amines condense to yield isomeric products [Co(dienbpe-1N)Cl](ZnCl4) (2) and [Co(dienbpe- 4N)Cl](ZnCl4) (3). Two of these (1 and 3) were characterized by single crystal x-ray crystallog. The corresponding reactions for the bis(pyridyl) ligand bpk {bis(pyridin-2-yl) ketone} provided C-N condensation products without the requirement for oxidation at the α-C center; two carbinolamine complexes in different geometrical configurations resulted, mer-anti-[Co(dienbpc)Cl]ZnCl4 (5) and unsym-fac-[Co(dienbpc)Cl]ZnCl4 (6), {dienbpc = [2-(2-aminoethylamino)-ethylamino]-di(pyridin-2-yl)methanol}. A novel complex, [Co(bpk)(bpd-OH)Cl]ZnCl4 (4), in which one bidentate N, N-bonded bpk ligand and one tridentate N,O,N-bonded bpd (the diol from bpk+OH-) were coordinated, was obtained via the Co(II)/O2 synthetic route. When the bpc ligand (bpc = bis(pyridin-2-yl)methanol) was employed directly as a reagent along with dien, no condensation reactions were observed, but rather a single isomeric complex [Co(dien)(bpc)]Cl.ZnCl4 (7), in which the ligand bpc acted as a N,N,O-bonded tridentate ligand rather than as a N,N-bidentate ligand was isolated. Carbon-13 and 1-dimensional and 2-dimensional 1H NMR studies are reported for all the complexes, which establish the structures unambiguously.

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 13 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN
ACCESSION NUMBER: 2004:958279 SCISEARCH Full-text
THE GENUINE ARTICLE: 864MI
TITLE: Synthesis and characterization of poly(3-acetyl-4-hydroxyphenyl acrylate) and its Cu(II) and Ni(II) complexes
AUTHOR: Nanjundan S (Reprint); Selvamalar C S J; Jayakumar R
CORPORATE SOURCE: Anna Univ, Dept Chem, Sardar Patel Rd, Madras 600025, Tamil Nadu, India (Reprint); Anna Univ, Dept Chem, Madras 600025, Tamil Nadu, India
snanjundan@yahoo.com

COUNTRY OF AUTHOR: India
SOURCE: EUROPEAN POLYMER JOURNAL, (OCT 2004) Vol. 40, No. 10, pp. 2313-2321.
ISSN: 0014-3057.
PUBLISHER: PERGAMON-ELSEVIER SCIENCE LTD, THE BOULEVARD, LANGFORD LANE, KIDLINGTON, OXFORD OX5 1GB, ENGLAND.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 42
ENTRY DATE: Entered STN: 25 Nov 2004
Last Updated on STN: 25 Nov 2004
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB 3-Acetyl-4-hydroxyphenyl acrylate (AHPA) was synthesized by treating acryloyl chloride with 2,5-dihydroxy acetophenone in the presence of triethylamine at 0 degreesC. AHPA was polymerized in ethyl methyl ketone (EMK) at 70 degreesC by free radical polymerization under nitrogen atmosphere using benzoyl peroxide as initiator. The monomer and the polymer were characterized by FT-IR, H-1-NMR and C-13-NMR spectroscopy. The polymer metal complexes were obtained by the reaction of chloroform solution of poly(AHPA) with aqueous solution of Cu(II)/Ni(II) acetates. The polymer-metal complexes were characterized by FT-IR and the results revealed that the ligands are coordinated through the oxygen of the keto group and oxygen of the phenolic -OH group to the metal ions. The electronic spectra and magnetic moment of polymer-metal complexes showed an distorted octahedral and square planar structure for poly(AHPA)-Ni(II) and poly(AHPA)-Cu(II) complexes respectively. The X-ray diffraction studies revealed that while the polymer was amorphous the polymer-metal complexes were crystalline . The thermal stability and glass transition temperature of the polymer-metal complexes were found to be higher than that of the polymer. (C) 2004 Elsevier Ltd. All rights reserved.

L8 ANSWER 5 OF 13 EMBASE COPYRIGHT (c) 2006 Elsevier B.V. All rights reserved on STN
ACCESSION NUMBER: 2004135966 EMBASE Full-text
TITLE: Recent kinase and kinase inhibitor x-ray structures: Mechanisms of inhibition and selectivity insights.
AUTHOR: Cherry M.; Williams D.H.
CORPORATE SOURCE: D.H. Williams, Sareum Ltd., 61 Cow Lane, Cambridge CB1 5HB, United Kingdom. david.williams@sareum.co.uk
SOURCE: Current Medicinal Chemistry, (2004) Vol. 11, No. 6, pp. 663-673. .
Refs: 50
ISSN: 0929-8673 CODEN: CMCHE7
COUNTRY: Netherlands
DOCUMENT TYPE: Journal; General Review
FILE SEGMENT: 015 Chest Diseases, Thoracic Surgery and Tuberculosis
016 Cancer
029 Clinical Biochemistry
030 Pharmacology
037 Drug Literature Index
LANGUAGE: English
SUMMARY LANGUAGE: English
ENTRY DATE: Entered STN: 12 Apr 2004
Last Updated on STN: 12 Apr 2004

AB Recent years have seen an explosion in the number of publicly available x-ray crystal structures of protein kinases. These structures have provided a wealth of information on the regulatory mechanisms, conformational plasticity and drugability of this important family of enzymes. Drawing upon structural information, new insights into the development of protein kinase inhibitors are discussed including de-novo design, molecular templates for ATP competitive inhibitors and alternative mechanisms of inhibition. The highly conserved nature of the ATP binding site is of central concern to drug development and the concept of a selectivity profile has arisen with structure-based design emerging as a key tool for addressing the challenges of specificity. In addition, protein-ligand complexes, where the enzyme is in an inactive conformation, signify an alternate approach to protein kinase inhibition. The belief that an inactive kinase presents a less conserved target is reviewed using observations on the structural changes occurring during protein kinase regulation. .COPYRGT. Bentham Science Publishers Ltd.

L8 ANSWER 6 OF 13 EMBASE COPYRIGHT (c) 2006 Elsevier B.V. All rights reserved on STN
ACCESSION NUMBER: 2004149172 EMBASE Full-text
TITLE: Preface.
AUTHOR: Bussiere D.E.
CORPORATE SOURCE: D.E. Bussiere, Biopharma Research, Chiron Corporation, Emeryville, CA, United States
SOURCE: Current Pharmaceutical Design, (2004) Vol. 10, No. 10, pp.

xxx. .
Refs: 6
ISSN: 1381-6128 CODEN: CPDEFP
COUNTRY: Netherlands
DOCUMENT TYPE: Journal; Editorial
FILE SEGMENT: 005 General Pathology and Pathological Anatomy
008 Neurology and Neurosurgery
016 Cancer
029 Clinical Biochemistry
030 Pharmacology
037 Drug Literature Index
LANGUAGE: English
ENTRY DATE: Entered STN: 22 Apr 2004
Last Updated on STN: 22 Apr 2004
DATA NOT AVAILABLE FOR THIS ACCESSION NUMBER

L8 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:154451 CAPLUS Full-text
DOCUMENT NUMBER: 138:183126
TITLE: Crystal structure of the kinase domain of murine Bruton's tyrosine kinase and its use for rational drug design of modulators.
INVENTOR(S): Uckun, Fatih M.
PATENT ASSIGNEE(S): Parker Hughes Institute, USA
SOURCE: PCT Int. Appl., 148 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003016338	A1	20030227	WO 2002-US26200	20020815
WO 2003016338	C2	20030731		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005196851	A1	20050908	US 2004-779399	20040213
PRIORITY APPLN. INFO.:			US 2001-312597P P	20010815
			US 2001-339206P P	20011207
			WO 2002-US26200 A1	20020815

AB The invention provides crystal structure of the kinase domain of Bruton's tyrosine kinase (BTK), as well as use of the crystal structure in the design, identification, and verification of ligands that modulate BTK activity. The x-ray crystal structure of the kinase domain of BTK (residues I397-S659) was determined by multiple isomorphous replacement, as well as BTK co-crystallized with a the Igα peptide ligand (NL*YEGL). The crystal has an orthorhombic space group symmetry, P212121, and includes unit cell dimensions of a = 45 ± 5, b = 104 ± 10, c = 116 ± 10 Å, α = β = γ = 90°. The 3-dimensional structure of BTK can be used for rational drug design, and for mapping the amino acid residues of mutations associated for X-linked agammaglobulinemia.
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 2001:846369 CAPLUS Full-text
DOCUMENT NUMBER: 136:17241
TITLE: Crystal structure of Bruton's tyrosine kinase domain suggests a novel pathway for activation and provides insights into the molecular basis of X-linked agammaglobulinemia
AUTHOR(S): Mao, Chen; Zhou, Min; Uckun, Faith M.
CORPORATE SOURCE: Department of Structural Biology, Parker Hughes Cancer Center, St. Paul, MN, 55113, USA
SOURCE: Journal of Biological Chemistry (2001), 276(44), 41435-41443
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology

DOCUMENT TYPE: Journal
LANGUAGE: English
AB Bruton's tyrosine kinase (I) is intimately involved in signal transduction pathways regulating survival, activation, proliferation, and differentiation of B lineage lymphoid cells. Mutations in the human btk gene are the cause of X-linked agammaglobulinemia, a male immune deficiency disorder characterized by a lack of mature, Ig-producing B lymphocytes. Here, the authors determined the x-ray crystal structure of the kinase domain of I in its unphosphorylated state to 2.1 Å resolution A comparison with the structures of other tyrosine kinases and a possible mechanism of activation unique to I were provided.
REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 9 OF 13 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN
ACCESSION NUMBER: 2001:719443 SCISEARCH Full-text
THE GENUINE ARTICLE: 468VZ
TITLE: Molecular determinants in pleckstrin homology domains that allow specific recognition of phosphoinositides
AUTHOR: Lemmon M A (Reprint); Ferguson K M
CORPORATE SOURCE: Univ Penn, Sch Med, Dept Biochem & Biophys, Philadelphia, PA 19104 USA (Reprint)
COUNTRY OF AUTHOR: USA
SOURCE: BIOCHEMICAL SOCIETY TRANSACTIONS, (AUG 2001) Vol. 29, Part 4, pp. 377-384.
ISSN: 0300-5127.
PUBLISHER: PORTLAND PRESS, 59 PORTLAND PLACE, LONDON W1N 3AJ, ENGLAND
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 63
ENTRY DATE: Entered STN: 21 Sep 2001
Last Updated on STN: 21 Sep 2001
ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS
AB More than 250 pleckstrin homology (PH) domains have been identified in the human proteome. All PH domains studied to date appear to bind phosphoinositides, most binding only weakly and non-specifically. Members of a small subclass of PH domains show both high affinity and specificity for particular phosphoinositides, and recent structural studies have provided detailed views of these specific interactions. We discuss the architecture of the specific phosphoinositide-binding sites of PH domains, and how selectivity can be modulated by sequence changes.

L8 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:434047 CAPLUS Full-text
DOCUMENT NUMBER: 127:160102
TITLE: Structure of the PH domain and Btk motif from Bruton's tyrosine kinase: molecular explanations for X-linked agammaglobulinemia
AUTHOR(S): Hyvonen, Marko; Saraste, Matti
CORPORATE SOURCE: European Molecular Biology Laboratory, Heidelberg, 69012, Germany
SOURCE: EMBO Journal (1997), 16(12), 3396-3404
CODEN: EMJODG; ISSN: 0261-4189
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Bruton's tyrosine kinase (Btk) is an enzyme which is involved in maturation of B cells. It is a target for mutations causing X-linked agammaglobulinemia (XLA) in man. We have determined the structure of the N-terminal part of Btk by X-ray crystallog. at 1.6 Å resolution This part of the kinase contains a pleckstrin homol. (PH) domain and a Btk motif. The structure of the PH domain is similar to those published previously: a seven-stranded bent β-sheet with a C-terminal α-helix. Individual point mutations within the Btk PH domain which cause XLA can be classified as either structural or functional in the light of the three-dimensional structure and biochem. data. All functional mutations cluster into the pos. charged end of the mol. around the predicted binding site for phosphatidylinositol lipids. It is likely that these mutations inactivate the Btk pathway in cell signalling by reducing its affinity for inositol phosphates, which causes a failure in translocation of the kinase to the cell membrane. A small number of signalling proteins contain a Btk motif that always follows a PH domain in the sequence. This small module has a novel fold which is held together by a zinc ion bound by three conserved cysteines and a histidine. The Btk motif packs against the second half of the β-sheet of the PH domain, forming a close contact with it. Our structure opens up new ways to study the role of the PH domain and Btk motif in the cellular function of Btk and the mol. basis of its dysfunction in XLA patients.

L8 ANSWER 11 OF 13 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on

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ACCESSION NUMBER: 1998:73026 SCISEARCH Full-text
THE GENUINE ARTICLE: YR382
TITLE: Structures and magnetic properties of some Fe(III) complexes with hexadentate ligands: in connection with spin-crossover behavior
AUTHOR: Hayami S (Reprint); Matoba T; Nomiyama S; Kojima T; Osaki S; Maeda Y
CORPORATE SOURCE: Kyushu Univ, Fac Sci, Dept Chem, Higashi Ku, Fukuoka 81281, Japan (Reprint); Kyushu Univ, Radioisotope Ctr, Higashi Ku, Fukuoka 81281, Japan
COUNTRY OF AUTHOR: Japan
SOURCE: BULLETIN OF THE CHEMICAL SOCIETY OF JAPAN, (DEC 1997) Vol. 70, No. 12, pp. 3001-3009.
ISSN: 0009-2673.
PUBLISHER: CHEMICAL SOC JAPAN, 1-5 KANDA-SURUGADAI CHIYODA-KU, TOKYO, 101, JAPAN.
DOCUMENT TYPE: Article; Journal
LANGUAGE: English
REFERENCE COUNT: 29
ENTRY DATE: Entered STN: 1998
Last Updated on STN: 1998

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

AB Several iron(III) complexes with the different hexadentate Schiff-base ligands of N4O2 donor sets were synthesized; these are 1 : 2 condensation products of linear tetramines (3,3,3-, 3,2,3-, 2,3,2- or 2,2,2-tetramine) and salicylaldehyde, acetophenone or benzophenone derivatives. Their crystal structures, Mossbauer spectra, magnetic susceptibilities, electronic spectra and cyclic voltammetry of the complexes were examined. The X-ray structures of the single crystals of [Fe(3,2, 3-sal(2)tet)]NO3 (1), [Fe(3,2,3-sal(2)tet)]BPh4 (2), [Fe(3,2,3-mpk(2)tet)]PF6 (3), [Fe(2,3,2-sal(2)tet)]ClO4 (4), [Fe(2,3,2-3MeO-sal(2)tet)]ClO4 (5), [Fe(2,3,2-mpk(2)tet)]ClO4 (6), [Fe(2,3,2-bpk(2)tet)]CLO4 (7), and [Fe(2,2,2-bpk(2)tet)]ClO4 . EtOH (8) were determined. Crystal data for (1): C22H28N5O5Fe, space group P2(1)/c, Z = 4, a = 7.607(1), b = 16.063(1), c = 19.063(1) Angstrom, beta = 91.00(2)degrees, V = 2329(3) Angstrom(3), R = 5.8%, R-w = 4.2%, 4605 reflections. Crystal data for (2): C46H48N4O2BFe, space group P2(1)/n, Z = 4, a = 14.390(6), b = 20.617(8), c = 14.754(5) Angstrom, beta = 115.85(2)degrees, V = 3939(2) Angstrom(3), R = 6.3%, R-w = 6.7%, 7458 reflections. Crystal data for (3): C24H32N4O2PF6Fe, space group P2(1)/c, Z = 4, a = 9.37(6), b = 24.15(7), c = 12.85(3) Angstrom, beta = 97.7(3)degrees, V = 2880(17) Angstrom(3), R = 10.9%, R-w = 13.6%, 5569 reflections. Crystal data for (4): C21H26N4O6ClFe, space group Pbcn, Z = 4, a = 11.041(2), b = 17.251(2), c = 11.722(2) Angstrom, V = 2232(1) Angstrom(3), R = 3.9%, R-w = 2.8%, 2258 reflections. Crystal data for (5): C23H30N4O8ClFe, space group Peen, Z = 8, a = 14.567(1), b = 22.288(1), c = 15.477(1) Angstrom, V = 5025(4) Angstrom(3), R = 6.2%, R-w = 6.2%, 4956 reflections. Crystal data for (6): C23H30N4O6ClFe, space group Pbca, Z = 8, a = 28.249(4), b = 13.989(4), c = 13.174(4) Angstrom, V = 5205(1) Angstrom(3), R = 8.2%, R-w = 8.4%, 5148 reflections. Crystal data for (7): C33H34N4O6ClFe, space group <P(1)over bar>, Z = 2, a = 10.241(3), b = 17.373(1), c = 9.692(7) Angstrom, alpha = 105.95(6)degrees beta = 91.61(4)degrees, gamma = 93.83(4)degrees, V = 1652(1) Angstrom(3), R = 7.1%, R-w = 7.6%, 6179 reflections. Crystal data for (8): C34H38N4O7ClFe, space roup P2(1)/c, Z = 4, a = 14.553(4), b = 14.079(4), c = 16.959(6) Angstrom, beta = 94.92(3)degrees, V = 3461(1) Angstrom(3), R = 8.4%, R-w = 7.7%, 6651 reflections: The moieties of the iron atoms of (1), (2), and (3) with 3,2,3-tetramine, and (7) with 2,3,2-tetramine were pseudo octahedral with trans-FeN4O2 geometry. Those of (4), (5), and (6) with 2,3,2-tetramine, and (8) with 2,2,2-tetramine were cis-FeN4O2 geometry. The iron(III) complexes (1), (2), (3), and (7) were in the low-spin state, and the iron(III) complexes (4), (5), (6), and (8) were in the high-spin state. In the electronic spectra, the wave lengths of the LMCT bands for the low spin complexes were longer than those for the high-spin complexes. The values of redox potentials for the low-spin states were suggested to be 0.12 V more negative than those for the high-spin states.

L8 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:544133 CAPLUS Full-text
DOCUMENT NUMBER: 113:144133
TITLE: The metal promoted hydration of di-2-pyridyl ketone: UV-visible spectra of copper(II) and chromium(III) in aqueous solution with di-2-pyridyl ketone and the x-ray structure analysis of bis(2,2',N,N'-bipyridyl ketone hydrate)chromium(III) chloride and ruthenium
AUTHOR(S): Sommerer, Shaun; Jensen, William P.; Jacobson, Robert A.
CORPORATE SOURCE: Dep. Chem., South Dakota State Univ., Brookings, SD, 57007, USA
SOURCE: Inorganica Chimica Acta (1990), 172(1), 3-11

CODEN: ICHAA3; ISSN: 0020-1693
DOCUMENT TYPE: Journal
LANGUAGE: English

AB [CrL2]Cl.4H2O and [RuL2].8H2O (I; HL = 2,2'-N,N'-bipyridyl ketone hydrate) were prepared and their crystal structures determined by x- ray methods. Crystal data are: monoclinic space group C2/c, Z = 4; triclinic space group P.hivin.1, Z = 1, resp. In both cases hydration occurs across the bipyridyl ketone (BPK) double bond in the ligand and one of the hydrate O atoms bonds to the metal to form a tridentate chelate. UV-visible spectra of solns. of Cu(II) and Cr(III) with BPK, reveal that initial coordination of BPK and the metal is rapid but that weeks are required to form the complex compds. that crystallize from solution The absorption spectra are shown to be pH dependent. An approx. correlation between off-axis angles of the coordinated O atoms and the difference between square planar and octahedral crystal field stabilization energy in 10 reported BPK hydrate complexes is indicated.

L8 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1965:484861 CAPLUS Full-text
DOCUMENT NUMBER: 63:84861
ORIGINAL REFERENCE NO.: 63:15642e-h
TITLE: Kinetics and mechanism of the transition of metastable tetragonal to monoclinic zirconia
AUTHOR(S): Whitney, E. Dow
CORPORATE SOURCE: Carborundum Co., Niagara Falls, NY
SOURCE: Transactions of the Faraday Society (1965), 61(513;Pt. 9), 1991-2000
CODEN: TFSOA4; ISSN: 0014-7672
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The time-dependency of the transition of spectroscopically pure metastable ZrO2, prepared via the thermal decomposition of ZrOCl2.4H2O at .apprx.500°, was investigated by x-ray diffraction techniques. Isothermal transition curves were obtained at 522-650°. The conversion curves do not exhibit any indication of an induction period. At .apprx.580° the transition rate is particularly rapid; >600° and <550° the transformation rate diminishes. The kinetic data do not comply with the conventional 1st-, 2nd-, or 3rd-order rate equations, but can be fitted reasonably well by Avrami's equation (CA 35, 31373), 1 - f(t) = exp(-Atk), where f(t) is the fraction of tetragonal ZrO2 transformed in time t, A is a constant, and k is the kinetic law exponent, obtained by plotting log {1/[1 - f(t)]} vs. log t. The constant A is related to the number of potential monoclinic nuclei and to the rate of formation and rate of growth of monoclinic growth nuclei, whereas k is related to the mechanism of growth of monoclinic nuclei in the tetragonal host matrix. The value of k varies from 0.40 to 0.14 over 522-50°. A value of k would equal 1/2, if complete edgewise impingement of thin plates occurs at an early stage of their precipitation Such a situation may exist in the transformation of tetragonal to monoclinic ZrO2 at .apprx.520°. The rapid drop in the value of k near 580° may in turn be due to a rapid formation of very small thin plates of monoclinic ZrO2, with the time necessary to reach complete edgewise impingement decreasing with increasing temperature The concept of a high nucleation rate, in the early stages of reaction at least, is supported by the apparent absence of an initial induction period in the isothermal transformation curves. The transition data can also be treated as a special case of Honig's application of order disorder theory to diffusionless transformation in solids (CA 54, 6243h). The rate constant calculated from order-disorder considerations exhibits a maximum with temperature in accordance with qual. deductions from the absolute reaction rate theory.

=> log y